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INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Sheet 1 of (

Complete if Known	
Application Number	10/053,348
Filing Date	November 2, 2001
First Named Inventor	Rosenthal, Dan E.
Art Unit	2123
Examiner Name	Unassigned
Attorney Docket Number	020910-000310US

OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS			
Examiner Initials *	Cite No.[1]	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T[2]
		ABAGYAN, et al., "*New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 2. Local Deformation Cycles*", 1989, Journal of Biomolecular Structure & Dynamics 6(4):833-845.	
		GIBSON, et al., "*Variable Step Molecular Dynamics: An Exploratory Technique for Peptides with Fixed Geometry*", 1990, Journal of Computational Chemistry 11(4):468-486.	
		JAIN, et al., "*Linearization of Manipulator Dynamics Using Spatial Operators*", 1993, IEEE Transactions on Systems, Man and Cybernetics 23(1):239-248.	
		LUDOVICE, et al., "*Molecular dynamics of geometrically constrained polymer systems in generalized coordinates: Basic formalism*", 1991, Computational Polymer Science 1:69-79.	
		MAZUR, et al., "*New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 1. Non-Cyclic Structures*", 1989, Journal of Biomolecular Structure & Dynamics 6(4):815-832.	
		PESKIN, ET AL., "*Molecular Dynamics by the Backward-Euler Method*", 1989, Communications on Pure and Applied Mathematics XLII:1011-1031.	
		ROSENTHAL, et al., "*High Performance Multibody Simulations via Symbolic Equation Manipulation and Kane's Method*", 1986, The Journal of the Astronautical Sciences, 34(3):223-239.	
		ROSENTHAL, "*An Order n Formulation for Robotic Systems*", 1990, The Journal of the Astronautical Sciences, 38(4):511-529.	
		ROSENTHAL, "*Engineers Notes: Triangulation of Equations of Motion for Robotic Systems*", 1988, The Journal of Guidance, 11(3):278-281.	
		SCHLICK, et al., "*A molecular dynamics simulation of a water droplet by the implicit Euler/Langevin scheme*", 1991, J. Chem. Phys., 94(3):2118-2129.	
		ZHANG, et al., "*The Langevin/implicit-Euler/normal-mode scheme for molecular dynamics at large timesteps*", 1994, J. Chem. Phys. 101(6):4995-5012.	

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JFR	AA	US 6,512,997	1/28/2003	Padilla, et al.	
	AB	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AC	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
	AD	US 6,125,235	9/26/2000	Padilla, et al.	
	AE	US 6,081,766	6/27/2000	Chapman, et al.	
	AF	US 6,014,449	1/11/2000	Jacobs, et al.	
	AG	US 5,787,279	7/28/1998	Rigoutsos	
	AH	US 5,777,889	7/7/1998	Mohanty, et al..	
	AI	US 5,752,019	5/12/1998	Rigoutsos, et al.	
	AJ	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AK	US 5,625,575	4/29/1997	Goyal, et al.	
	AL	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
JFR	AM	US 5,307,287	4/26/1994	Cramer, III, et al.	

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JFR	AN	WO	02/073334	A2	07-26-1990	Padilla, et al.		☐
JFR	AO	WO	01/67310	A1	12-12-1991	Smith, et al.		☐
JFR	AP	WO	96/24902	A1	04-01-1993	Wertz		☐

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JFR	AQ	ASCHER, et al., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
JFR	AR	BARAFF, et al., "*Large steps in cloth simulation*", 1998, Computer Graphics Proceedings SIGGRAPH 98 (Orlando, July 19-24) p43.pdf	
JFR	AS	BARTH, et al., "*A separating framework for increasing the timestep in molecular dynamics*" in Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3, 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	

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JSP ✓	AT	BERENDSEN, "*Molecular Dynamics Simulations: The Limits and Beyond*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 3-36, Springer-Verlang, Germany.	
✓	AU	BISCHOF, et al., ADIFOR 2.0 Users' Guide, 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
✓	AV	BRENAN, et al., Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
✓	AW	BUTCHER, "*Towards efficient implementation of singly-implicit methods*", 1988, AMC Transactions of Mathematical Software 14:68-75.	
✓	AX	BYSTROFF, "*An alternative derivation of the equations of motion in torsion space for a branched linear chain*", 2001, Protein Engineering 14:825-828.	
✓	AY	COLEMAN, et al., "*The efficient computation of sparse Jacobian matrices using automatic differentiation*", 1996, Cornell Theory Center Technical Report CTC95TR225.	
	AZ	EICHBERGER, et al., "*The benefits of parallel multibody simulation*", 1994, International Journal for Numerical Methods in Engineering, 37:1557-1572.	
✓	BA	GOLUB, et al., "*The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate*", 1973, SIAM J. Numer Anal. 10:413.	
✓	BB	✓ HAIRER, et al., Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, 2nd ed., 1996, Springer-Verlang, Germany.	
✓	BC	HE, et al., "*Macromolecular conformational dynamics in torsional angle space*", 1998, Journal of Chemical Physics 108:271.	
✓	BD	HOLLARS, et al., SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamics, California.	
✓	BE	IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, J.Chem.Phys. 110:9853.	
	BF ✓	KANE, Dynamics, 3rd ed., 1978, Stanford University, Stanford, California.	
JSP	BG ✓	LEACH, Molecular Modelling Principles and Applications, 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	

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Sheet 3 of 3

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JPM	BH	MARTINS, et al., "*An automated method for sensitivity analysis using complex variables*", 2000, American Institute of Arenautics and Astronoautics, 2000-0689 p1	
	BI	NORSETT, et al., "*Embedded SDIRK-methods of basic order three*", 1984, BIT 24:634-646.	
	BJ	PONDER, TINKER User's Guide, Version 3.8, October 2000, Washington University, St. Louis, MO.	
	BK	RAPAPORT, The Art of Molecular Dynamics Simulation, 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
	BL	SCHLICK, "*Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation*", 1997, Annu. Rev. Biophys. Biomol. Struct., 26:181-222.	
	BM	SCHLICK, "*Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 227-262, Springer-Verlang, Germany.	
	BN	SCHLICK, Molecular Modeling and Simulation - An Interdisciplinary Guide, 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlang, Germany.	
	BO	SHAMPINE, "*Implementation of implicit formulas for the solution of ODEs*", 1980, SIAM J. Sci. Stat. Comput. 1:103-118.	
	BP	VERLET, "*Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*", 1967, Physical Review, 159(1):98-103.	
	BQ	VON SCHWERIN, Multibody System Simulation, 1999, Springer-Verlang, Germany.	
	BR	WU, et al., "*Constraint dynamics algorithm for simulation of semiflexible macromolecules*", 1998, Journal of Computational Chemistry 19:1555-1566	
JPM	BS	YEN, et al., "*On the numerical solution of constrained multibody dynamic systems*", 1994, University of Minnesota AHPCRC 94-038.	

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JSR	AA	US-6,253,166 B1	06-26-2001	Whitmore et al.	
JSR	AB	US-6,150,179	11-21-2000	Went	
JSR	AC	US-5,799,312	08-25-1998	Rigoutsos	

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JP	AD	MOROKUMA et al., "Model studies of the structures, reactivities, and reaction mechanisms of metalloenzymes," IBM J. Res. & Dev., 45(3/4):367-395 (2001).	

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JJO	AA	5,424,963		Turner et al.	06-13-1995	
JJO	AB	5,249,151		Chang et al.	09-28-1993	

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JSR	AC	LEUNG et al., "Concurrent DASSL: A Second-Generation DAE Solver Library," IEEE Proceedings of Scalable Libraries Conference, from conference held 10/6-8/93 at Syracuse University, New York, NY, pgs. 204-210.	
JSR	AD	ABDEL-RAHMAN et al., "Determination of the Ligamentous and Contact Forces in the Human Tibio – Femoral Joint Using a Three – Dimensional Dynamic Anatomical Model," IEEE Proceedings of Biomedical Engineering Conference, from conference held 3/29-31/96 in Dayton Ohio, pgs. 373-376.	

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